Specification of Collective Submanifold  
by Adiabatic Time-Dependent Hartree-Fock Method
--- Coupled Lipkin Model ---

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With the use of adiabatic time-dependent Hartree-Fock method, a collective submanifold is specified for the case of the coupled Lipkin model. The energy spectra, which belong to those of collective mode, are well reproduced with the aid of the canonical quantization.

The (adiabatic) time-dependent Hartree-Fock method (TDHF) is the most promising candidate for the microscopic description of large amplitude collective motions. Mukherjee and Pal, however, have pointed out that the equation of collective submanifold derived by the ordinary adiabatic TDHF does not always guarantee a unique specification of collective submanifold even with the aid of the RPA boundary condition. This is based on the singularity in the differential equation at the stationary point of the potential energy surface. In their discussion, further, they regarded the canonical-variable condition usually called the weak canonicity condition as the one determining the mass of collective motion. On the other hand, we have recently shown the following facts: The basic set of equations, such as the equation of collective submanifold and the canonical-variable condition, is invariant under any canonical transformation of collective variables. The mass of collective motion is originally dependent on the choice of the collective coordinate system. Considering that the collective submanifold itself does not depend on the choice of its canonical coordinate system, we can select it properly, for instance, by demanding that the mass of collective motion becomes one. Further, by requiring certain analytic property of the collective submanifold in the neighbourhood of the stationary point of the potential energy surface, we have a possibility of selecting out a unique solution of the equation of collective submanifold.

In this note, we determine the collective submanifold with the aid of adiabatic TDHF for the coupled Lipkin model investigated by Hayashi and Iwasaki and show how well the resultant collective Hamiltonian can reproduce the energy spectra belonging to the collective mode with the aid of the canonical quantization.

We start with the definition of the coupled Lipkin model. The Hamiltonian is given by

\[ H = \sum_{\sigma} \hat{H}_{\sigma} - V_0(S_1+\bar{S}_2+S_2+\bar{S}_1), \]

\[ \hat{H}_{\sigma} = 2\varepsilon_{\sigma} \hat{S}_{\sigma} - \frac{1}{2} V_0(S_{\sigma} + \bar{S}_{\sigma}), \]

where the quasi-spin operators are defined as

\[ S_{\sigma} = \sum_{m=-j}^{j} \hat{a}_{\sigma m} \hat{a}_{\sigma m}^\dagger (-)^{j-m} b_{\sigma m}^\dagger, \]

\[ \hat{S}_{\sigma} = \hat{S}_{\sigma}, \]

\[ \hat{S}_{\sigma} = 2 \sum_{m=-j}^{j} (\hat{a}_{\sigma m} \hat{a}_{\sigma m}^\dagger + \hat{b}_{\sigma m} \hat{b}_{\sigma m}^\dagger) - \Omega; \]

\[ \Omega = j + \frac{1}{2}. \]

In this note, we consider only the collective motion within the subspace of zero seniority number. Hence, the classical image of the above system can be obtained with the aid of TDHF, where the Slater determinantal state is specified with the use of the prescription given by Baranger and Veneroni. Then, the quasi-spin operators are transcribed in the following forms in terms of a certain set of canonical variables \((q, p)\):

\[ S_{q} = \frac{1}{2} (S_{\sigma} + S_{\sigma}) = \Omega \sqrt{1 - \tilde{p}_\sigma^2} \sin q^\sigma, \]

\[ S_{p} = \frac{1}{2} (S_{\sigma} - S_{\sigma}) = -\Omega \tilde{p}_\sigma, \]

\[ S_{q} = S_{p} = -\Omega \sqrt{1 - \tilde{p}_\sigma^2} \cos q^\sigma; \quad \tilde{p}_\sigma = p_\sigma / \Omega. \]

The Hamiltonian can be given as

\[ H = \sum_{\sigma} \hat{H}_{\sigma} - V_0(S_1 + S_2 + S_2 + \bar{S}_1), \]

\[ H_{\sigma} = -\Omega [2\varepsilon_{\sigma} \sqrt{1 - \tilde{p}_\sigma^2} \cos q^\sigma]. \]
+ V_0(Q - \frac{1}{2})(1 + \sin^2 q^\sigma) \times \{ (1 - \tilde{p}_\sigma^2) \sin^2 q^\sigma - \tilde{p}_\sigma^2 \}. \quad (4b)

In the classical form, the system is described in a 4-dimensional symplectic manifold, the coordinate system of which is provided by the set of variables \((q, p)\). The geometry of this manifold is specified by the Poisson bracket

\[
\{ A, B \}_{(q, p)} = \sum_{\alpha=1}^{2} (\partial_{\alpha} A \cdot \partial_{\alpha} B - \partial_{\alpha} A \cdot \partial_{\alpha} B). \quad (5)
\]

Then, the classical images of quasi-spin operators satisfy the following Poisson brackets, which just correspond to the quantal commutation relations:

\[
[S_{\alpha}, S_{\alpha}^l]_{(q, p)} = i\delta_{\alpha l} S_{\alpha k} \delta_{k l}, \quad k, l = x, y, z. \quad (6)
\]

Then, we can go back to the original quantal system with the aid of the canonical quantization:

\[
[S_q, S_p]_{(\Omega, P)} = \frac{\hbar}{2} \delta_{kl} S_{k\Omega}^l, \quad \{ S_q, S_p \}_{(\Omega, P)} = \frac{\hbar}{2} \delta_{kl} S_{k\Omega}^l. \quad (7a)
\]

\[
[S_p, S_q]_{(\Omega, P)} = -\frac{\hbar}{2} S_{k\Omega}^l, \quad \{ S_p, S_q \}_{(\Omega, P)} = -\frac{\hbar}{2} S_{k\Omega}^l. \quad (7b)
\]

In the above, the degeneracy \(\Omega\) is replaced by \(\Omega' = \Omega + \frac{1}{2}\), in order to take into account the quantum fluctuation effect.

Here, we give the equation of collective submanifold prescribed by TDHF in the following form:\n
\[
\partial_{\Omega} H = \lambda \partial_{\rho} \rho - \mu \partial_{\rho} \rho, \quad \partial_{P} H = -\lambda \partial_{\rho} q^\sigma + \mu \partial_{\rho} q^\sigma, \quad \frac{1}{2} \sum_{\alpha=1}^{2} (\partial_{q^\sigma} \rho \cdot \partial_{q^\sigma} \rho - \partial_{q^\sigma} \rho \cdot \partial_{q^\sigma} \rho) = 1. \quad (8)
\]

Equation (8) is called the equation of collective submanifold and Eq. (9) is the canonical-variable condition for collective variables \((Q, P)\). These equations are invariant under any canonical transformation of \((Q, P)\). In order to specify a canonical coordinate system suitable for the adiabatic treatment, we put the following condition:\n
\[
\sum_{\alpha=1}^{2} p^\alpha \cdot \partial_{\rho} q^\sigma = P, \quad \sum_{\alpha=1}^{2} p^\alpha \cdot \partial_{\rho} q^\sigma = 0. \quad (10)
\]

Equation (9) can be easily derived from Eq. (10). Hence, the basic set of equations consists of Eqs. (8) and (10) within TDHF.

In spite of conditions (10), the collective coordinate system cannot be fixed, since Eq. (10) is still invariant under any point transformation such as

\[
Q' = Q'(Q), \quad P' = \frac{dQ}{dQ'} P. \quad (11)
\]

As was shown in Ref.2), therefore, we can fix it by demanding that the mass of collective motion becomes one.

Till now, the discussion is given within the framework of TDHF. Now we introduce the adiabatic approximation which corresponds to the lowest order approximation when we express the various relations such as Eqs. (8) and (10) in terms of a power series with respect to \(P\).\n
Under this approximation, \(q\) and \(p\) are expressed in the forms:

\[
q^\sigma = q^\sigma(Q), \quad p^\sigma = p^\sigma(Q)P. \quad (12)
\]

Corresponding to the above approximation, the starting Hamiltonian takes the following form:

\[
H = \frac{1}{2} \sum_{\sigma} M^{\sigma\sigma} p^\sigma p^\sigma + V(q), \quad (13a)
\]

\[
M^{\sigma\sigma} = \left[ 2 \varepsilon \cos q^\sigma + 2 V_0 \left( Q - \frac{1}{2} \right) \sin^2 q^\sigma \right]/Q' + 2 V_0 \sin q^\sigma \sin q^\sigma, \quad (13b)
\]

\[
M^{\sigma\sigma} = -2 V_0 \sin \frac{1}{2}, \quad (13c)
\]

where we take into account the quantal fluctuation effect since we must quantize the system after all.

Then, the basic set of equations is reduced to the forms:

\[
\frac{d\rho^\sigma(Q)}{dQ} = \partial_{\rho} V, \quad (14a)
\]

\[
\sum_{\sigma} \rho^\sigma(Q) \frac{d\rho^\sigma(Q)}{dQ} = 1. \quad (14b)
\]

The second of Eq. (10) is automatically satisfied under the approximation (12) and Eq. (14a) obtained from the first of Eqs. (10) becomes identical with that derived from Eq. (9). Hence, the above basic set is completely equivalent to that of the ordinary adiabatic TDHF. Contrary to the ordinary approach, however, we regard the collective mass to be determined properly in order to fix the collective coordinate system. In the
above, we put it equal to one.

Here, we note the following relation derived from Eqs. (14a) with the aid of Eq. (14b):

\[ C(Q)Q = \partial Q\partial V. \]  

(15)

By solving Eq. (14), we can determine \( C(Q) \). Hence, the collective Hamiltonian is given by

\[ H_c = \frac{1}{2} \dot{q}^2 + V_c(Q); \]

\[ V_c(Q) = \int_q^Q C(Q')Q'dQ'. \]  

(16)

On the other hand, the collective potential energy \( V_c(Q) \) can be also given by

\[ V_c(Q) = V(q(Q)). \]  

(17)

Therefore, we can use the coincidence between the above two potential energies in order to check the accuracy of the present numerical calculation.

We solve Eqs. (14) in the following forms:

\[ q^n(Q) = \sum_{n=0}^{\infty} q_n Q^{2n+1}, \quad \rho_n(Q) = \sum_{n=0}^{\infty} \rho_n Q^{2n}, \]

\[ C(Q) = \sum_{n=0}^{\infty} C_n Q^{2n}. \]  

(18)

As the boundary condition, we adopt the RPA boundary condition to fix the lowest order terms in expansions (18).

In this note, we give a preliminary numerical results in order to show how well the present prescription works in the specification of collective submanifold and the resultant collective Hamiltonian can reproduce the energy spectra belonging to the collective mode. In the numerical calculation, we adopt the following set of values for various parameters:

\[(\epsilon_1, \epsilon_2) = (1.5, 2.0), \]

\[(V_1, V_2, V_3) = (0.05\chi, 0.1\chi, 0.075\chi), \quad \Omega = 5. \]  

(19)

which is that adopted in Ref.4). For the check of the validity, we investigate some typical cases, a rather stable normal case, a transitional and a rather stable super case.

In Fig. 1, we give the resultant collective path for the above three cases. In case that the above power series becomes an alternative one, we simulate it by a certain rational function, i.e., by the Padé approximation. In Fig. 2, we give the collective potential energy obtained from the second of Eq. (16) and also that of Eq. (17). Both of these potential energies coincide with each other, when we solve Eq. (14) exactly. In the well-overlapped region at least, therefore, we can safely use the collective Hamiltonian obtained

\[ \text{Fig. 1. Collective path and contour plot of potential energy } V(q). \text{ Three illustrative cases are given: (a) } x=1.0, \text{ (b) } x=2.0, \text{ (c) } x=4.0. \text{ The curves of collective path are plotted for the region } (-3,3) \text{ of collective coordinate } Q. \text{ This region is sufficient for estimating excitation energies of low-lying collective excited states.} \]

\[ \text{Fig. 2. Collective potential energy.} \]

The broken lines denote the collective potential energy \( V_c(Q) \) defined by Eq. (16) and the solid ones express \( V(q(Q)) \) defined by Eq. (17). The coincidence between the two implies the accuracy of the present approximation.
Fig. 3. Energy spectra of collective motion.
For each force strength, the leftmost expresses the exact energy spectra, the middle is the present numerical result and the rightmost is the result given in Ref. 8. Levels denoted by solid line belong to even-parity states and those of broken ones to odd-parity states.

under the present approximation. Thus, we can treat the ground and the relatively lower excited states in the normal, in the transitional and in the super region.

The collective Hamiltonian given by Eq. (16) can be easily quantized by the canonical quantization. The calculated energy spectra are given in Fig. 3, together with exact ones belonging to the collective mode. For the comparison, we give also the results obtained with the use of TDHF by one of the present authors (A. K.). From this figure, we can see that the present prescription on the basis of the adiabatic TDHF works well in the specification of collective submanifold and also in the reproduction of the collective energy spectra.

In the super region, we cannot pick up definitely the collective energy levels for rather higher excited states only by looking the energy systematics. Hence, we give in Fig. 3 two possible candidates for $\chi = 4.0$. In the succeeding paper, we will discuss the collective properties of each excited state in more details.